JS 9/30/21
RJA 01/03/22

Chemistry Report for Case # P-16-0400

General

Submitter: Shell Chemical LP

Contact: Melissa Bourque

Contact Telephone No.: (713) 241-2719

TS No.: 201602

Chemist: Roberts, Justin

Contractor Support: Y

PV Init (kg/yr): 15000000.0000

PV Max (kg/yr): 63500000.0000

Binding Option: ☐

Exposure-Based Review: ☑

Manufacture: ☐

Import: ☑

CAS Number: 1809170-78-2

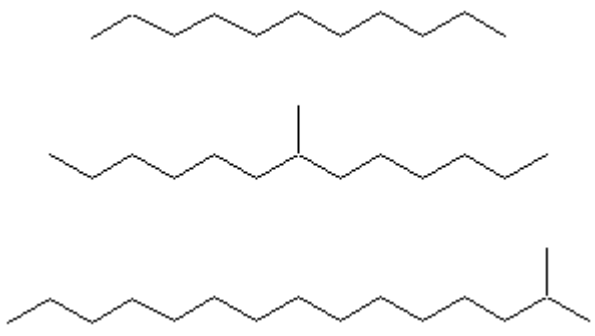
Chemical Name: Alkanes, C11-16-branched and linear

Trade Name: GTL Solvent GS1927, GS9127

IES Order: 396548

Generic Name: not CBI

Chemical Structure



Physical Chemical Properties

Molecular Weight: 156.31

Molecular Formula:C11 H24	
% < 500:	**% < 1000:**
MP:	**MP Estimate:**<-25
BP:	**BP Pressure:**760.00
BP Estimate:	
VP (Torr):	**VP Estimate (Torr):**0.27
Water Solubility (g/L):	**Water Soluble Estimate (g/L):**0.000004
Log P:	**Log P Estimate:**5.74
Physical State — Neat: Liquid	**Physical State — Manuf:**NK - Imported

Physical State — Processing: Solution, 70% PMN material in coatings or 5% in cleaning fluids or 45% in agrochemical formulation or 35% in metalworking fluid or used neat as a chem

Physical State — End Use: Solution or Destroyed

Additional Chemical Info

The structures drawn are representative. The number and positions of the branching are variable and unspecified. The PMN material consists of 60-85% (typical 76%) iso-paraffins and 15-40% (typical 24%) n-paraffins, with <10% (typical 0%) C10, <15% (4.7% typical) C11, 10-25% (22.1% typical) C12, 10-30% (typical 24.2%) C13, 15-30% (typical 28.2%) C14, 10-30% (typical 16%) C15, 2-15% (typical 4.6%) C16, and <5% (typical 0.1%) C17+. Submitted data: BP = 212.1 to 258.2 °C; VP = 0.15 torr (est.); insoluble in water; log P = 4.5-7; flash point = 70 °C, > 78 °C; auto ignition temp. = 200 °C, > 200 °C; 515 mg/kg aromatics (0.0515%, as determined by UV analysis); density = 0.764 at 15 °C; refractive index = 1.428; aniline point = 87 °C; viscosity = 2.4 mm2/s at 25 °C, 1.8 mm2/s at 40 °C; kinematic viscosity < 0.2 mm2/s at 25 °. IR, MS, UV/Vis, and 1H-NMR spectra are included with the PMN submission. Additional data on page 6. NOMO5 estimated data from BP of 212.1 to 258.2°C: VP = 0.024 to 0.27 torr. Measured data for representative low weight component (top structure as drawn), [redacted] (PhysProp): MP = -25.6 °C; BP = 195.9 °C; VP = 0.412 torr; WS = 4.4E-6 g/L; log P = 5.74 (EPI est.). EPI estimated data for representative

typical component (middle structure as drawn), 7-methyltridecane, [redacted]: MP = -37.2 °C (meas., PhysProp); BP = 232 °C; VP = 0.108 torr; WS = 1.17E-5 g/L; log P = 7.14. EPI estimated data for representative high weight component, 2-methylpentadecane (bottom structure as drawn): BP = 267 °C; VP = 0.0182 torr; WS = 1.25E-6 g/L; log P = 8.13. Data for feedstock Distillates (Fischer-Tropsch), C8-26-branched or linear [redacted]: The position and degree of branching is unspecified. 50% of the C8 alkanes are linear and 50% are branched. As the carbon numbers increase, the % branching increases to 95% branched at C26. The carbon number distribution is 0.40% C8, 2.70% C9, 4.92% C10, 7.64% C11, 7.77% C12, 7.73% C13, 7.81% C14, 7.71% C15, 7.47% C16, 7.53% C17, 7.12% C18, 6.98% C19, 6.39% C20, 5.92% C21, 4.77% C22, 3.67% C23, 2.40% C24, 1.00% C25 and 0.07% C26.

Uses

Consumer Use? No

Use: Solvent/diluent in coatings (25%), cleaning fluids (9.5%), agrochemicals (3.2%), and metalworking fluids/rolling oils (8.9%), and as a chemical intermediate (53.4%).

Other Uses: [redacted]

Reaction Description

The PMN material is produced via factional distillation of Distillates [redacted]

Pollution Prevention Analysis(P2 Analysis:)

P2 Claims: This PMN Submission is the subject of a P2 Assessment for participation in the Sustainable Futures Initiative. The P2 assessment of Hydrocarbons, C11-16, branched and linear, with CAS RN 1809170-78-2, referred to as SHL003 in the assessment, directly follows this cover letter. Additional model outputs and methods for all the P2 framework

tools used in this assessment can be provided upon request. SHL003 is an inherently low hazard substance. Extensive testing of similar GTL Solvent mixtures has shown little to no human health effects for the substances. In addition, aquatic effects testing has shown that similar alkyl mixtures with alkyl ranges of C10 and greater show low acute and chronic effects to the aquatic environment. These results are collected in a summary reference below and attached to the PMN; they also cover previous PMNs, including P-14-132 to P-14-137, that showed for both human health and ecotoxicity concerns, EPA concurs that the hazard levels were low for alkyl ranges consisting of C10 or greater. Based on this, SHL003 is predicted to have a low human health cancer and non-cancer hazard concerns, as well as low aquatic toxify hazard concerns. SHL003 is predicted to partition primarily to air and soil, where it will have a low concern for persistence, with an environmental half-life of <2 days in air and <60 days in all other media The conclusion of the SHL003 aquatic risk assessment is that, based on low hazard, there is a low potential for risk to the aquatic environment. The conclusion of the SHL003 occupational and general population risk assessments is that, based on low hazard predicted for the substance, there is a low potential for risk to human health. It should be noted that this risk assessment does not take PPE and other exposure controls into account when determining exposure and risk. These factors would further reduce the potential for risk from this substance. It is our opinion that based on this assessment of the chemical and information included in the PMN submission and manufacturer's MSDS, including use of appropriate PPE and exposure controls, SHL003 will not pose an unreasonable risk to human health or the environment.

Analogs

Analogs:
[redacted]

Comments/Telephone Log

Artifact	Update/Upload Time
[redacted]	[redacted]